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ANL/NDM-82

Reaction Differential Cross Sections from the Least-Squares Unfolding of Ratio Data Measured in Diverse Neutron Fields

by

Donald L. Smith

January 1984

ARGONNE NATIONAL LABORATORY,
ARGONNE, ILLINOIS 60439, U.S.A.

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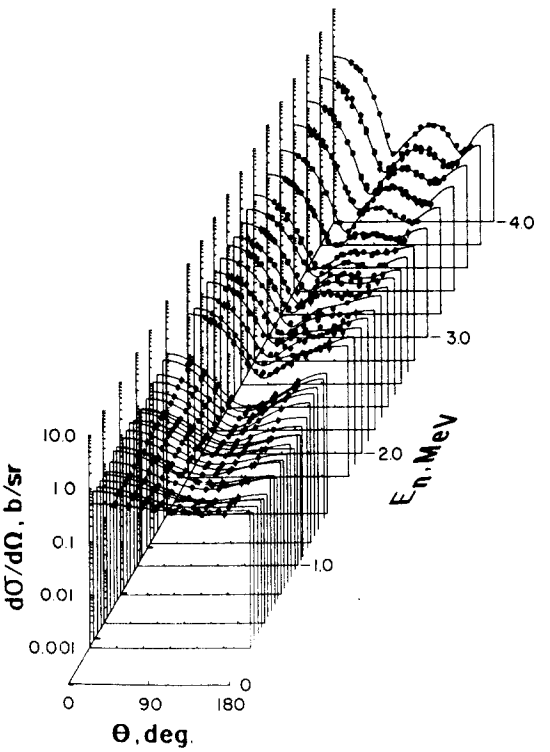

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COVARIANCE MATRIX METHODOLOGY. Least-squares technique. Thick-target neutrons. Integral ratio data unfolding. Differential cross section derivation. A priori cross sections. Evaluation technique. Simulated experiment.

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REACTION DIFFERENTIAL CROSS SECTIONS FROM THE LEAST-SQUARES UNFOLDING OF RATIO DATA MEASURED IN DIVERSE NEUTRON FIELDS*

by

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ABSTRACT

A previously-described procedure for deriving threshold reaction differential cross sections from integral measurements in well-specified neutron fields by means of least-squares unfolding is extended to the analysis of ratio data. The following information is required for the least-squares analysis of ratio data: i) shape specifications for the neutron spectra and the associated uncertainties and correlations, ii) standard reaction group cross section values and their covariance matrix, iii) the ratio data and their covariance matrix, and iv) the a priori group cross sections and their covariance matrix. Knowledge of the absolute neutron fluence is not required. In order to illustrate this method, a special class of ratio measurements is investigated in detail and numerical analysis is performed for a hypothetical simulated experiment.

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I. INTRODUCTION

The concept of extracting differential cross section information for a threshold reaction from measured response data for well-characterized broad-spectrum neutron fields has been described in a previous report (Ref. 1). An important feature of this earlier development is that the quantities Φ, which collectively provide a group representation for a particular set of such neutron spectra, must be absolutely normalized.

It is well known that one can more readily determine neutron spectral shapes than their absolute normalizations. In the more familiar domain of monoenergetic measurements one often resorts to ratio experiments to avoid the problem of fluence normalization. Consequently, in the present report the procedure described in Ref. 1 is applied to the analysis of reaction ratio measurements. The objective here is the same as it was earlier, namely to improve upon current knowledge of a specific reaction cross section by performing integral measurements. Now, the integral spectra need no longer be normalized, although the shapes must be well known. Instead, knowledge of the differential cross section for a standard reaction is required.

The formalism required for this approach is developed in Section II. It is seen that although the algebra is tedious, the methodology is a straightforward extension of that presented in Ref. 1. In order to fully comprehend the content of the present work, the reader will find it necessary to refer on various occasions to this earlier work. The symbols here are altered only to the extent needed to distinguish quantities which are physically different from those in Ref. 1, although they play corresponding roles in the formulas from Ref. 1. For convenience, those formulas which

have counterparts in Ref. 1 are often labelled with the equation numbers from Ref. 1 (in braces {...}) as well as with the sequential equation numbers of the present report. The greatest challenge in the present development is in keeping track of appropriate subscripts. The present development is sufficiently detailed so that the reader can follow most new steps in the analysis without performing extra algebra to fill the gaps.

The meanings of the general formulas derived in Section II are not readily transparent. Therefore, a special case is treated in some detail in Section III to help the reader to understand the material. This case treats a series of essentially monoenergetic ratio measurements. A corresponding hypothetical numerical example is also presented in order to demonstrate the method.

II. FORMALISM

The starting point for the present analysis is Eq. {32} from Ref. 1. Actually this represents m distinct equations which provide a model that relates a set of integral responses a_i (i = 1,m) to group representations for m well-characterized spectra Φ_i (i = 1,m) and the differential cross section σ. There, σ and all the Φ_i are vectors of dimension n. The vector elements are group values as discussed in Ref. 1.

Here, however, we wish to examine what can be learned about the cross section σ from a set of integral ratio measurements r_i (i = 1,m) involving a second cross section s which is assumed to be a standard. Eq. {32} from Ref. 1 is not directly applicable in this situation. The r_i can be considered to have been derived from

$$r_i = (a_i/b_i) \quad (i = 1,m) \quad , \tag{1}$$

where

$$a_i = \sum_{k=1}^{n} \phi_{ik}\sigma_k = \Phi_i^+ \cdot \sigma \qquad (i=1,m) \quad , \qquad (2) \quad \{32\}$$

$$b_i = \sum_{\ell=1}^{n} \phi_{i\ell}\, s_\ell = \Phi_i^+ \cdot s \qquad (i=1,m) \quad . \qquad (3) \quad \{32\}$$

Here, all the symbols play roles analagous to Ref. 1. The b_i represent integral response values for the standard reaction. The s_ℓ ($\ell = 1,n$) are group cross sections for the standard, and together they form the vector s. Eq. (1) becomes a problem if any of the b_i equal zero. Consequently, the neutron energy limits (E_ℓ, E_h) and the selected group structure are established so that the energy interval encompasses the response ranges for both the cross section we wish to improve (σ) and the standard (s). We assume that both reactions have thresholds and that the standard has the lower threshold. Then none of the b_i will vanish.

Combining Eqs. (1)-(3) yields the result

$$r_i = (\Phi_i^+ \cdot \sigma)/(\Phi_i^+ \cdot s) \qquad (i = 1,m) \quad . \qquad (4)$$

We chose to use the following alternate nomenclature in much of the analysis below:

$$I_{\sigma i} = a_i = (\Phi_i^+ \cdot \sigma) \qquad (i = 1,m) \quad , \qquad (5)$$

$$I_{si} = b_i = (\Phi_i^+ \cdot s) \qquad (i = 1,m) \quad . \qquad (6)$$

Then we can write

$$r_i = I_{\sigma i}/I_{si} = \sum_{k=1}^{n} (\phi_{ik}/I_{si})\sigma_k \qquad (i = 1,m) \quad . \qquad (7)$$

If ψ_i (i=1,m) are defined as m vectors with the elements

$$\psi_{ik} = \phi_{ik}/I_{si} \qquad (i = 1,m; \quad k=1,n) \quad , \tag{8}$$

then

$$r_i = \sum_{k=1}^{n} \psi_{ik}\, \sigma_k = \Psi_i^{+} \cdot \sigma \qquad (i = 1,m) \quad . \tag{9}$$

The ψ_{ik} serve essentially as normalized group fluxes, with the normalization constants deduced from response factors for the standard reaction. The formalism appearing between Eq. {32} and Eq. {54} in Ref. 1 is entirely applicable now, provided that we make the following explicit substitutions of variables:

$$\begin{aligned}
&\Phi \rightarrow \Psi \quad , \\
&A_o \rightarrow R_o \quad , \\
&A \rightarrow R \quad , \\
&N_{Ao} \rightarrow N_{Ro} \quad , \\
&N_A \rightarrow N_R \quad , \\
&N_A^{\sigma} \rightarrow N_R^{\sigma} \quad , \\
&N_A^{\Phi} \rightarrow N_R^{\Psi} \quad .
\end{aligned} \tag{10}$$

Ψ is the collection of all the ψ_{ik} and it can be treated either as an (m,n) matrix or as a vector of dimension $q = m \times n$. There is a one-to-one relationship between Ψ and Φ, as is evident from Eq. (8). R_o is the vector of experimental ratio values (m of them), and R represents the corresponding calculated ratios, according to the model defined by Eq. (7). N_{Ro} and N_R are the corresponding covariance matrices. N_R^{σ} and N_R^{Ψ} are two additional matrices to be defined later in this report.

There is no need to repeat the entire development appearing in pp. 11-16 of Ref. 1; however, the present equivalents to Eqs. {46}-{54} are worthy of reproduction for they are the formulas actually used in practical analytical

applications. Thus, paraphrasing Ref. 1, we define c_{ij} by

$$r_i = \sum_{j=1}^{n} c_{ij} \qquad (i = 1,m) \quad , \tag{11} \{46\}$$

$$c_{ij} = \psi_{ij}\sigma_j \qquad (i=1,m;j=1,n) \quad .$$

Then

$$N_R = N_R^{\sigma} + N_R^{\psi} \quad , \tag{12} \{47\}$$

where

$$(N_R^{\sigma})_{ij} = \psi_i^{+} \cdot N_{\sigma} \cdot \psi_j$$

$$= \sum_{k=1}^{n} \sum_{\ell=1}^{n} \psi_{ik}(N_{\sigma})_{k\ell}\, \psi_{j\ell} \qquad (i,j = 1,m), \tag{13} \{48\}$$

$$(N_R^{\psi})_{ij} = \sigma^{+} \cdot N_{\psi ij} \cdot \sigma$$

$$= \sum_{k=1}^{n} \sum_{\ell=1}^{n} \sigma_k\, (N_{\psi ij})_{k\ell}\, \sigma_{\ell} \qquad (i,j = 1,m). \tag{14} \{49\}$$

N_{σ} is an (n,n) matrix while N_{ψ} is a (q,q) matrix (remember that $q = m \times n$). $N_{\psi ij}$ is a submatrix of N_{ψ} with dimension (n,n); there are m^2 such submatrices in N_{ψ}. Here, as in Ref. 1, the nomenclature $(Q)_{k\ell}$ designates a specific element of any matrix (or submatrix) labelled Q.

A matrix V can be defined by

$$V = N_{Ro} + N_R = N_{Ro} + N_R^{\sigma} + N_R^{\psi}; \tag{15} \{50\}$$

it has dimension (m,m). This matrix is inverted to yield W (i.e., $W = V^{-1}$).

Now, define elements u_{ij} by

$$u_{ij} = \sum_{k=1}^{n} (N_\sigma)_{jk}\, c_{ik}/(\sigma_j \sigma_k) \qquad (i=1,m;\ j=1,n) \quad . \tag{16}$$ {51}

Then the solution σ' and covariance matrix N_σ' can be calculated using the formulas

$$\sigma_j' = \sigma_j \left[1 + \sum_{k=1}^{m} \sum_{\ell=1}^{m} u_{kj} w_{k\ell}\, (r_{o\ell} - r_\ell) \right] \quad (j=1,n), \tag{17}$$ {52}

$$(N_\sigma')_{ij} = (N_\sigma)_{ij} - \sigma_i \sigma_j \sum_{k=1}^{m} \sum_{\ell=1}^{m} w_{k\ell}\, u_{ki} u_{\ell j} \quad (i,j=1,n) \quad . \tag{18}$$ {53}

The $r_{o\ell}$ and r_ℓ are elements of R_o and R, respectively. The $w_{k\ell}$ are elements of the inverse matrix W. Also,

$$\chi_m^2 = \sum_{k=1}^{m} \sum_{\ell=1}^{m} (r_{ok} - r_k) w_{k\ell}\, (r_{o\ell} - r_\ell) \quad . \tag{19}$$ {54}

Although the formulas are essentially identical to the corresponding ones in Ref. 1, matters are not quite as simple as they appear. The problem is that the covariance matrix N_Ψ, or its equivalent collection of submatrices $N_{\Psi ij}$ (i,j=1,m), is as yet unspecified. These submatrices must be known in order to evaluate Eq. (14). The remaining job, therefore, is to develop a formula for the elements $(N_{\Psi ij})_{k\ell}$ in terms of other known quantities.

This problem is a straightforward but tedious exercise in error combination, as described in Refs. 2 and 3. A good approach is to consider the entire set Ψ of elements ψ_{ik} as a single vector of dimension q=n × m. For any given pair (i,k) of subscripts which identify an element of Ψ, there is a unique α which corresponds to it. This unique equivalence relationship is symbolized by

$$(i,k) \leftrightarrow \alpha \qquad (i=1,m; k=1,n; \alpha=1,q) \quad . \tag{20}$$

Thus we can make the explicit symbol exchanges

$$\psi_{ik} \sim \psi_\alpha \qquad (i=1,m;k=1,n;\alpha=1,q) \tag{21}$$

for convenience. By definition, Ψ depends only on Φ and s, so

$$\psi_\alpha = \psi_\alpha(\Phi,s) \quad (\alpha = 1,q) \quad . \tag{22}$$

Here, we also treat Φ as a vector of dimension q, as discussed above. The covariance matrix $N\psi$ can be calculated according to the uncertainty combination rules described in Section IV of Ref. 2. Since there are no correlations assumed between the uncertainties for Φ and s, we can write

$$\begin{aligned}(N\psi)_{\alpha\beta} = {} & (S_{\alpha\phi} \cdot E_\phi)^+ \cdot C_\phi \cdot (S_{\beta\phi} \cdot E_\phi) \\ & + (S_{\alpha s} \cdot E_s)^+ \cdot C_s \cdot (S_{\beta s} \cdot E_s) \quad (\alpha,\beta = 1,q) \quad ,\end{aligned} \tag{23}$$

where $S_{\alpha\phi}$, $S_{\beta\phi}$, $S_{\alpha s}$ and $S_{\beta s}$ are sensitivity matrices, E_ϕ and E_s are uncertainty vectors, and C_ϕ and C_s are correlation matrices, according to the definitions from Ref. 2.

As an entirely equivalent alternative to Eq. (23), we consider the more convenient formula (for present purposes)

$$(N\psi)_{\alpha\beta} = Z_{\alpha\phi}^+ \cdot N_\phi \cdot Z_{\beta\phi} + Z_{\alpha s}^+ \cdot N_s \cdot Z_{\beta s} \quad (\alpha,\beta = 1,q) \; . \tag{24}$$

$Z_{\alpha\phi}$ and $Z_{\beta\phi}$ are sensitivity vectors of dimension q. $Z_{\alpha s}$ and $Z_{\beta s}$ are sensitivity vectors of dimension n. N_ϕ is the (q,q) dimension covariance matrix for Φ and N_s is the (n,n) dimension covariance matrix for s.

The matrix N_s must be a part of the input to the problem along with the standard reaction group cross sections s. The matrix N_ϕ might be generated as described on p. 16 of Ref. 1, i.e., it might be possible to calculate it using Eqs. {55}-{57} from that reference. This leaves us with only one remaining task, namely derivation of the Z-vectors.

The elements of $Z_{\alpha\phi}$ are the partial derivatives $(\partial\psi_\alpha/\partial\phi_\lambda)$ for α=1,q and λ=1,q. For each λ there is a unique pair (i',k'). Thus

$$(i',k') \sim \lambda \quad , \tag{25}$$

so

$$\frac{\partial \psi_\alpha}{\partial \phi_\lambda} \rightarrow \frac{\partial \psi_{ik}}{\partial \phi_{i'k'}} \qquad (\alpha,\lambda=1,q) \tag{26}$$

Referring to Eqs. (5), (6) and (8) one sees that

$$(Z_{\alpha\phi})_\lambda = \frac{\partial \psi_\alpha}{\partial \phi_\lambda} = \delta_{ii'}\, I_{si}^{-2}\, (I_{si}\, \delta_{kk'} - \phi_{ik} s_{k'}). \tag{27}$$

Typical elements of the vector $Z_{\beta\phi}$ are the partial derivatives $(\partial\psi_\beta/\partial\phi_\rho)$ for $\beta = 1,q$ and $\rho = 1,q$. Assuming the subscript equivalence relations

$$\beta \rightarrow (j,\ell) \quad , \tag{28}$$

and

$$\rho \rightarrow (j',\ell') \quad , \tag{29}$$

it is readily seen by analogy to Eq. (27) that

$$(Z_{\beta\phi})_\rho = \frac{\partial \psi_\beta}{\partial \phi_\rho} = \delta_{jj'}\, I_{sj}^{-2}\, (I_{sj}\, \delta_{\ell\ell'} - \phi_{j\ell} s_{\ell'}) \tag{30}$$

Eqs. (25)-(30) together yield an expression for the first term in Eq. (24):

$$\begin{aligned} Z_{\alpha\phi}^{+} \cdot N_\phi \cdot Z_{\beta\phi} &= \sum_{\lambda=1}^{q} \sum_{\rho=1}^{q} \left(\frac{\partial \psi_\alpha}{\partial \phi_\lambda}\right) (N_\phi)_{\lambda\rho} \left(\frac{\partial \psi_\beta}{\partial \phi_\rho}\right) \\ &= \sum_{i'=1}^{m} \sum_{j'=1}^{m} \sum_{k'=1}^{m} \sum_{\ell'=1}^{n} \delta_{ii'}\delta_{jj'} I_{si}^{-2} I_{sj}^{-2} (I_{si}\delta_{kk'} - \phi_{ik}s_{k'})\, (N_{\phi i'j'})_{k'\ell'} \\ &\quad \cdot (I_{sj}\, \delta_{\ell\ell'} - \phi_{j\ell} s_{\ell'}) \\ &= I_{si}^{-2} I_{sj}^{-2} \sum_{k'=1}^{n} \sum_{\ell'=1}^{n} (I_{si}\, \delta_{kk'} - \phi_{ik} s_{k'})\, (N_{\phi ij})_{k'\ell'}\, (I_{sj}\, \delta_{\ell\ell'} - \phi_{j\ell} s_{\ell'}). \end{aligned} \tag{31}$$

The elements of $Z_{\alpha s}$ are the partial derivatives $(\partial\psi_\alpha/\partial s_{k'})$ for $\alpha=1,q$ and $k'=1,n$. Thus,

$$(Z_{\alpha s})_{k'} = \left(\frac{\partial\psi_\alpha}{\partial s_{k'}}\right) = - I_{si}^{-2}\, \phi_{ik}\, \phi_{ik'} \quad . \tag{32}$$

Likewise for $Z_{\beta s}$ we have

$$(Z_{\beta s})_{\ell'} = \left(\frac{\partial\psi_\beta}{\partial s_{\ell'}}\right) = - I_{sj}^{-2}\, \phi_{j\ell}\, \phi_{j\ell'} \quad . \tag{33}$$

Thus, the second term from Eq. (24) is

$$Z_{\alpha s}^{+} \cdot N_s \cdot Z_{\beta s}$$

$$= I_{si}^{-2} I_{sj}^{-2} \sum_{k'=1}^{n} \sum_{\ell'=1}^{n} \phi_{ik}\phi_{ik'}(N_s)_{k'\ell'}\phi_{j\ell}\phi_{j\ell'} \quad . \tag{34}$$

Eqs. (31) and (34) can be combined with Eq. (24). We also note from the preceding discussion that

$$(N_\psi)_{\alpha\beta} = (N_{\psi ij})_{k\ell} \quad . \tag{35}$$

Thus,

$$(N_{\psi ij})_{k\ell} = I_{si}^{-2} I_{sj}^{-2} \sum_{k'=1}^{n} \sum_{\ell'=1}^{n} \Big[\phi_{ik}\phi_{ik'}(N_s)_{k'\ell'}\phi_{j\ell}\phi_{j\ell'}$$

$$+ (I_{si}\delta_{kk'} - \phi_{ik}s_{k'})\,(N_{\phi ij})_{k'\ell'}(I_{sj}\delta_{\ell\ell'} - \phi_{j\ell}s_{\ell'}) \Big] . \tag{36}$$

Eq. (36) is the general result we have sought. We see that analysis of ratio data and inclusion of a standard cross section leads to considerably more calculational effort than is required for the topic considered in Ref. 1.

III. A SPECIAL CASE

Monoenergetic measurements form a subset of the ensemble of all possible integral measurements. In Ref. 1, no distinction is made between integral and monoenergetic spectra. None need be made in the present development either. By monoenergetic we will simply mean that for a particular spectrum all the neutrons are in a single group. This particular category of problem was chosen to exemplify the present general method because the outcome is rather easy to comprehend when compared with a conventional approach to monoenergetic measurements which is likely to be familiar to most readers.

Consider the following special set of monoenergetic measurements:

$$\phi_{ik} = \delta_{ik}\phi_i \quad (i=1,n;\ k=1,n) \quad . \tag{37}$$

Here, m=n so there is one ratio value for each group considered. Eqs. (2) and (3) assume the forms

$$a_i = \phi_i\sigma_i \qquad (i=1,n) \quad , \tag{38}$$

$$b_i = \phi_i s_i \qquad (i=1,n) \quad , \tag{39}$$

and Eq. (1) becomes

$$r_i = (a_i/b_i) = \sigma_i/s_i \qquad (i=1,n) \quad . \tag{40}$$

Eqs. (37)-(40) reflect the obvious fact that for monoenergetic ratio measurements no knowledge at all of the spectral parameters ϕ_i is required. However, Ψ, as defined in Section II, must still be considered.

This problem, therefore, is only partially degenerate in the context of the formalism of Section II. In fact,

$$\psi_{ik} = \delta_{ik}/s_i \qquad (i=1,n;k=1,n) \quad . \tag{41}$$

We wish to see what form N_ψ assumes in this special case. Consider the general formula expressed in Eq. (36). In general N_ψ is a (q,q) matrix, as is N_ϕ, but the reader can easily convince himself (e.g., it can be done graphically) that for the present special case both N_ψ and N_ϕ have a true rank of n, not q. Thus

$$(N_{\psi ij})_{k\ell} = \delta_{ik}\delta_{j\ell}\,(N_{\psi ij})_{ij} \qquad (i,j,k,\ell=1,n) \quad , \tag{42}$$

$$(N_{\phi ij})_{k'\ell'} = \delta_{ik'}\delta_{j\ell'}(N_{\phi ij})_{ij} \qquad (i,j,k',\ell'=1,n) \quad . \tag{43}$$

Clearly from Eq. (6),

$$I_{si} = \phi_i s_i \qquad (i=1,n) \quad . \tag{44}$$

Substitution of Eqs. (41)-(44) into Eq. (36) leads to the expression:

$$(N_{\psi ij})_{ij} = (\phi_i s_i)^{-2}(\phi_j s_j)^{-2}\Big[\phi_i{}^2(N_s)_{ij}\phi_j{}^2 + (\phi_i s_i - \phi_i s_i)\,(N_{\phi ij})_{ij}\,(\phi_j s_j - \phi_j s_j)\Big] \qquad (i,j=1,n) \quad , \tag{45}$$

since $\delta_{ki}=\delta_{ik}$ and $\delta_{\ell j}=\delta_{j\ell}$ for all i,j,k and ℓ.
The second term of Eq. (45) vanishes for all i and j, regardless of N_ϕ, as we know it must. Since Ψ does not depend upon Φ in this special case, it is clear that N_ψ must not depend upon N_ϕ. Simplifying Eq. (45) yields

$$(N_{\psi ij})_{ij} = s_i{}^{-2}(N_s)_{ij}\,s_j{}^{-2} \qquad (i,j=1,n) \quad , \tag{46}$$

so

$$(N\psi_{ij})_{k\ell} = \delta_{ik}\delta_{j\ell}\, s_i^{-2}\, (N_s)_{ij} s_j^{-2} \qquad (i,j,k,\ell=1,n) \quad . \tag{47}$$

Refer to matrix V defined by Eq. (15). Combining the information in Eqs. (12)-(15) yields

$$(V)_{ij} = (N_{Ro})_{ij} + \sum_{k=1}^{n} \sum_{\ell=1}^{n} \psi_{ik}\, (N_\sigma)_{k\ell} \psi_{j\ell} + \sum_{k=1}^{n} \sum_{\ell=1}^{n} \sigma_k (N\psi_{ij})_{k\ell} \sigma_\ell \qquad (i,j=1,n) \quad . \tag{48}$$

Using Eqs. (41) and (47), this reduces to

$$(V)_{ij} = (N_{Ro})_{ij} + s_i^{-1}(N_\sigma)_{ij} s_j^{-1} + \sigma_i s_i^{-2} (N_s)_{ij}\, \sigma_j s_j^{-2} \qquad (i,j=1,n) \quad . \tag{49}$$

This form of V is the one which is inverted in the least-squares algorithm, as applied to the present special case.

For this special case, we can also arrive at the same mathematical formulas using the formalism directly from Ref. 1. Eq. {32} from Ref. 1 takes the form

$$r_i = \left(\frac{1}{s_i}\right)\sigma_i \qquad (i=1,n) \quad , \tag{50}$$

provided that we make the substitution

$$\phi_{ij} = (\delta_{ij}/s_i) \qquad (i=1,n; j=1,n) \quad . \tag{51}$$

We make the following additional substitutions also:

$$\varepsilon_i = s_i \quad (i=1,n) \quad , \tag{52}$$

$$\nu_{ij} = \delta_{ij} \quad (i,j=1,n) \quad , \tag{53}$$

$$f_{\nu ik} = 0 \quad (i,k=1,n) \quad , \tag{54}$$

$$(C_\varepsilon)_{k\ell} = (C_s)_{k\ell} \quad (k,\ell=1,n) \quad , \tag{55}$$

$$\Delta E_k = 0 \quad (k=1,n) \quad . \tag{56}$$

Then, from Eqs. {55} and {56} of Ref. 1, we have

$$\begin{aligned}(N_{\phi ij})_{k\ell} &= \phi_{ik}\phi_{j\ell}\,(C_\varepsilon)_{k\ell} f_{\varepsilon k} f_{\varepsilon \ell} \\ &= \delta_{ik}\, s_i^{-1}\delta_{j\ell} s_j^{-1}(C_s)_{k\ell}\, E_{sk}E_{s\ell}\, s_k^{-1}s_\ell^{-1} \\ &= \delta_{ik}\delta_{j\ell}\, s_i^{-2}(N_s)_{ij}s_j^{-2} \\ &\qquad (i,j,k,\ell=1,n) \quad ,\end{aligned} \tag{57}$$

which is equivalent to Eq. (47). Here, we also utilize the expressions

$$f_{\varepsilon k} = f_{sk} = E_{sk}/s_k \qquad (k=1,n) \quad , \tag{58}$$

$$(N_s)_{ij} = E_{si}(C_s)_{ij}\, E_{sj} \qquad (i,j=1,n) \quad , \tag{59}$$

which follow from standard formulas given in Ref. 2. The code UNFOLD (Appendix of Ref. 1) cannot be utilized in general for analysis of ratio results. However, it is apparent from an examination of Eqs. (50)-(59) that UNFOLD can be conveniently used for the special case discussed in this section. Therefore, for interest we demonstrate this special case with a simulated numerical example.

Numerical Example

Consider a ten-group problem (n=m=10). Each group is 250 keV broad and, as required, the groups are contiguous. Let σ be the true reaction

group cross section, s the true standard group cross section, and r the resultant ratios. Specific numerical values appear in Table 1. These values correspond to perfect (but unattainable) knowledge of the parameters of this problem.

Assume that values of the ratio r can be measured to 10% accuracy with 7% of the error correlated and 7% random. Thus, the off-diagonal correlations are 0.5. Based upon this assumption, we wish to generate a simulated set of "measured" ratio values r_{oi} (i=1,10). First, using a computer random number generator, we produce a table of random numbers in the interval (0,1) which is long enough for the present application. Table 2 is this requisite table. We select random numbers in sequence from this table, as required, and never use any number more than once. We must decide on the common "bias" factor for the set of r_{oi}. A correlated uncertainty of ± 7% implies that the "measured" set could be biased relative to the true ratios (Table 1) by a factor in the range 0.93 - 1.07. The first random number in Table 2 is 0.0957943794, so this leads to the bias factor 0.94341. Thus, we use the following formula to generate our "measured" r_{oi}:

$$r_{oi} = 0.94341\ (0.93 + 0.14\ R_i)r_i \qquad (i=1,10), \tag{60}$$

where the r_i come from Table 1 and R_1 through R_{10} are the next ten available random numbers from Table 2. This algorithm superimposes a ± 7% random fluctuation into the generation of the r_{oi} from the corresponding r_i. The final values r_{oi}, representing "measured" quantities, appear in Table 3.

Next, we generate a set of realistic standard cross sections s_{oi} which appropriately reflect the imperfect knowledge of the true standard cross sections, as given in Table 1. The procedure is very similar to the

one described in the preceding paragraph. For simulation purposes it is assumed that the standard cross section has a 5% uncertainty with 50% correlation between groups. This is equivalent to 3.5% systematic plus 3.5% random error. Using the next available random number from Table 2, which is 0.0125493309, we deduce a bias factor of 0.96588. Thus, the standard cross sections available for the unfolding procedure are assumed to be given by the formula

$$s_{oi} = 0.96588\ (0.965 + 0.07\ R_i')s_i \qquad (i=1,10) \tag{61}$$

where the s_i come from Table 1 and R_1' through R_{10}' are the next ten available random numbers from Table 2. Referring to the monoenergetic "measured" ratio values r_{oi} and the available standard cross sections s_{oi} (both from Table 3), one can deduce the set of cross sections ξ_{oi}, also given in Table 3, from the formula

$$\xi_{oi} = r_{oi}s_{oi} \qquad (i=1, 10)\ . \tag{62}$$

The ξ_{oi} are resultant "experimental" cross section values one would normally deduce from a monoenergetic experiment and available information for the standard cross section. It is seen that the derived ξ_{oi} in Table 3 are systematically lower in general than the corresponding true σ_i from Table 1. An examination of Eqs. (60)-(62) readily reveals the reason for this effect. Unfortunately for our hypothetical experimenter, the particular random numbers used to generate the bias factors for both r_{oi} and s_{oi} were such that both bias factors were smaller than unity, leading to a resultant bias factor for the ξ_{oi} of 0.91122 (~ 9% low). Such a bias factor is entirely possible given the 7% systematic uncertainty for the ratios r_{oi} and the 3.5% systematic uncertainty

for the standard cross section. Thus, the ξ_{oi} values derived by our hypothetical experimenter are entirely consistent with his imperfect knowledge of the standard and the accuracy of his ratio experiment. No matter how much one may wish matters to be otherwise, one cannot realistically expect to escape the ravages of uncertainty in any research endeavor.

Turning now to the least-squares algorithm, we require an a priori which represents the best available knowledge of σ before the present hypothetical investigation. Call σ_o that a priori, with the group values σ_{oi} as given in Table 4. Assume each σ_{oi} has a 25% uncertainty of which 10% is correlated between all the values. This corresponds to a correlation parameter of 0.16 between all the a priori values. The least-squares algorithm, as applied to the present special example, serves to generate essentially a properly weighted average between the "experimental" cross sections ξ_{oi} and the a priori cross sections σ_{oi}. The uncertainties for the ξ_{oi} are derived from the "measured" ratio and available standard cross section uncertainties. Owing to the correlations, the solution to this problem is rather more complicated than simple weighted averaging. The results of this analysis appear in Table 5. The solution group cross section is designated σ', and the solution covariance matrix N_σ' provides the information needed to obtain the errors and correlations which appear in Table 5. This analysis yields a value of 1.507 for χ^2_m, well within the acceptable range of 0.3-2 discussed in Ref. 1.

Fig. 1 summarizes the results of the present analysis in graphical form. The solution group cross sections σ' are closer to the true cross section σ than the a priori σ_o in most groups, but the results are still rather disappointing. However, in this hypothetical simulation we know the reason

for this, based on the preceding discussion. It would be naive to anticipate better agreement between σ' and σ in view of the assumed uncertainties in the ratio measurements and the imperfect knowledge of the standard cross sections. If the uncertainties in the "measured" ratios and in the standard cross sections had been smaller (say < 3%), and if the "measured" ratios and the available standard cross section values were actually consistent with the true values within these errors, then the algorithm would have assigned the a priori σ_o rather little weight and the solution σ' would have come much closer to the true σ. Clearly, a good ratio experiment involving a well-known standard will lead to results which essentially over-ride a much less accurate a priori result. As discussed in Ref. 1, difficulties might be encountered if the assumed uncertainty correlations for the a priori were large, and if the shape of the a priori were quite wrong. Such an eventuality would lead to a χ_m^2 beyond the range 0.3-2, thus providing warning that a serious inconsistency existed in the problem.

ACKNOWLEDGEMENT

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Table 1

Hypothetical True Group Values

Group i	E_i[a] (keV)	Range (keV)	σ_i[b] (mb)	s_i[c] (mb)	r_i
1	750	625-875	10	100	0.1
2	1000	875-1125	40	140	0.28571
3	1250	1125-1375	80	170	0.47059
4	1500	1375-1625	120	180	0.66667
5	1750	1625-1875	140	186	0.75269
6	2000	1875-2125	150	190	0.78947
7	2250	2125-2375	145	194	0.74742
8	2500	2375-2625	130	198	0.65657
9	2750	2625-2875	120	200	0.6
10	3000	2875-3125	110	202	0.54455

[a] Group midpoint energy.
[b] Reaction cross section group values.
[c] Standard cross section group values.
[d] $r_i = (\sigma_i/s_i)$ $(i=1,10)$.

Table 2

Computer-Generated Random Number Table[a]

1	.0957943794
2	.206700238
3	.280750548
4	.65063982
5	.870623822
6	.100842989
7	.782173608
8	.678838465
9	.0902449467
10	.257296116
11	.588115974
12	.0125493309
13	.928071414
14	.426676491
15	.362051404
16	.9033449
17	.666980722
18	.878140029
19	.223352529
20	.933383622
21	.047625462
22	.168465527
23	.399603901
24	.163556252
25	.664763506
26	.835937616
27	.701282477
28	.457966566
29	.13683168
30	.333691762
31	.109179255
32	.212207831
33	.10884974
34	.304091252
35	.548779062
36	.67559223
37	.507522759
38	.343729539
39	.0243280515
40	.93795434

[a] Random number table for the range (0,1) generated using an Apple IIe microcomputer.

Table 3

Hypothetical Available Group Values

Group i	R_i [a]	r_{oi}	R_i' [b]	s_{oi}	ξ_{oi} [c]
1	0.206700238	0.090467	0.928071414	99.482	8.9998
2	0.280750548	0.216127	0.426676491	134.53	35.149
3	0.65063982	0.45332	0.362051404	162.61	73.714
4	0.870623822	0.66158	0.9033449	178.77	118.27
5	0.100842989	0.67041	0.666980722	181.75	121.85
6	0.782173608	0.77422	0.878140029	188.37	145.84
7	0.678838465	0.72278	0.223352529	183.75	132.81
8	0.0902449467	0.58388	0.933383622	197.05	115.05
9	0.257296116	0.54681	0.047625462	187.06	102.29
10	0.588115974	0.52007	0.168465527	190.58	99.115

[a] Random numbers from Table 2 used in Eq. (60) to calculate r_{oi} values.
[b] Random numbers from Table 2 used in Eq. (61) to calculate s_{oi} values.
[c] $\xi_{oi} = r_{oi}s_{oi}$ $(i=1,10)$.

Table 4

Hypothetical A Priori Group Cross Sections

Group i	σ_{oi} (mb)
1	30
2	60
3	90
4	109
5	120
6	120
7	110
8	100
9	90
10	80

Table 5

Solution Cross Sections, Errors and Correlations

Group i	E_i[a] (keV)	σ_i'[b] (mb)	Error in σ_i'[b]	Error Correlations[b]									
				1	2	3	4	5	6	7	8	9	10
1	750	9.3537	17.6%	1									
2	1000	34.995	12.0%	0.41	1								
3	1250	71.769	10.7%	0.38	0.42	1							
4	1500	111.86	10.1%	0.34	0.40	0.42	1						
5	1750	116.19	10.2%	0.35	0.41	0.42	0.42	1					
6	2000	135.68	10.0%	0.33	0.40	0.41	0.42	0.42	1				
7	2250	123.69	10.0%	0.33	0.40	0.41	0.42	0.42	0.42	1			
8	2500	107.94	10.0%	0.34	0.40	0.42	0.42	0.42	0.42	0.42	1		
9	2750	96.133	10.1%	0.34	0.40	0.42	0.42	0.42	0.42	0.42	0.42	1	
10	3000	91.916	10.0%	0.33	0.40	0.41	0.42	0.42	0.42	0.42	0.42	0.42	1

[a]Group midpoint energy.

[b]Solution from unfolding algorithm.

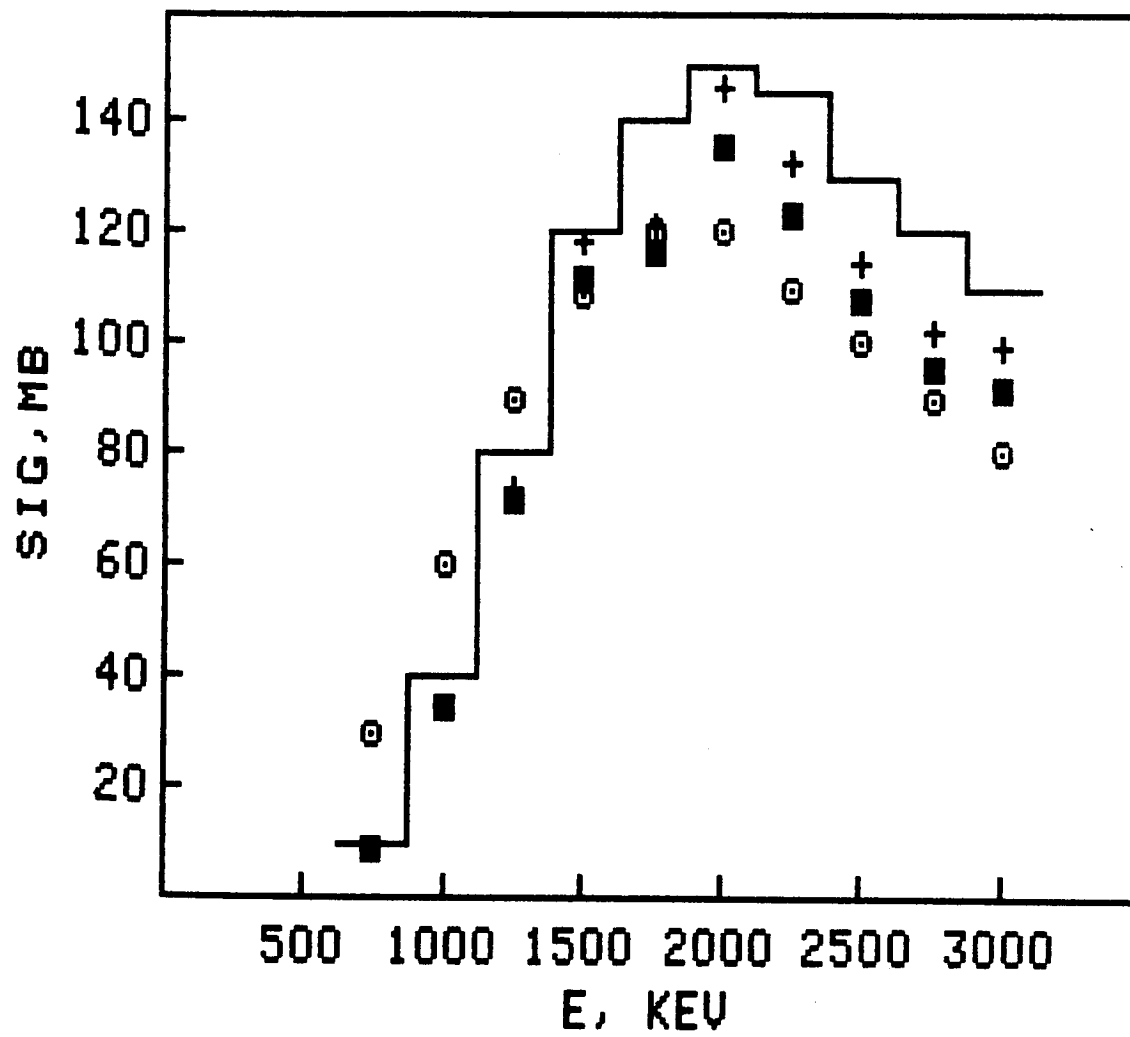

Figure 1: Plot of reaction group cross sections for hypothetical simulation: true cross section (⎽⎺), apriori cross section (⊙), measured cross section (+), and unfolded solution cross section (■). Error bars are not plotted so as to avoid cluttering the figure.